A Fragmentation Mechanism Of Homemade Explosive TMDD Using DART-MS And Isotopic Labeling

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Abstract

A fragmentation mechanism and characterization for the first time using Direct Analysis in Real Time-Time of Flight-Mass Spectrometry (DART-TOF-MS) of the tetramethylene diperoxide dicarbamide (TMDD) compound were presented. The MS-spectrum may support other research about devices and detection in real scene. The mass spectrum of TMDD obtained using DART ionization in the positive-ion detection mode exhibited a strong peak at m/z 254 representing an ammonium adduct ($[TMMD \cdot NH_4]^+$). There was another peak at m/z 237, which represented the protonated molecule ($[TMDD \cdot H]^+$) of TMDD. These two peaks corroborated the identity of the analyte. The DART-MS spectra of the TMDD-isotopomer successfully corroborated the respective molecular tails. The principal fragmentation residues also showed coherence according to the number of isotopically labeled atoms on the TMDD structure. In contrast with other organic peroxides analyzed by this technique, TMDD exhibited substantial fragmentation. The theoretical modeling results showed that the fragmentation mechanism of the TMDD ion adduct is strongly dependent of the TMDD ring flexibility and the hydrogen bonding formed between the nitrogen and oxygen atoms and the atmospheric proton.

Keywords

Direct Analysis In Real Time; Isotopomers; Time Of Flight-Mass Spectrometry; TMDD.